

Singular current response from isolated impurities in d -wave superconductors

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The current response of a d -wave superconductor containing a single impurity is calculated and shown to be singular in the low-temperature limit, leading in the case of strong scattering to a $1/T$ term in the penetration depth $\lambda(T)$ similar to that induced by Andreev surface bound states. For a small number of such impurities, we argue this low- T upturn could be observable in cuprate superconductors.

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Introduction. The quasiparticle excitations near the line nodes in the d -wave superconducting order parameter of the cuprate high- T_c materials lead to well-known singularities in the current response of such systems, resulting in nontrivial magnetic field dependences of the London penetration depth in the Meissner state[1], and of the specific heat in the Abrikosov vortex state[2]. These excitations are also responsible for the marginal thermodynamic stability of the d -wave state itself, which has been related[3, 4] to the famous linear- T temperature dependence of the penetration depth $\lambda(T)$ [5].

Recently, it has been pointed out by Walter et al.[6] and Barash et al.[7], that, in addition to effects arising from extended quasiparticle states alone, there are $1/T$ contributions to the penetration depth below a crossover temperature $T_{m0} \simeq \sqrt{\xi_0/\lambda_0}T_c$, where ξ_0 is the coherence length and T_c the critical temperature, due to zero-energy surface bound states. These states arise within a semiclassical picture when a quasiparticle reflected from the surface experiences a change of sign in the order parameter; the upturns therefore only occur when the surface normal of the sample makes an angle close to $\pi/4$ with the crystal axes and hence the antinodal directions of the d -wave order parameter. A $\lambda(T) \sim 1/T$ term in the penetration depth has in fact been reported by Carrington et al.[8], and attributed to the paramagnetic current carried by such states which dominates at low T . The field and interface angle dependence also appear to be in rough agreement with the predictions of Barash et al.[7]. Upturns correlated with disorder introduced by Zn atoms observed by Bonn et al.[9] seem to vary from sample to sample, and are not currently understood.

Most works in this area have treated disorder within effective-medium approximations which predict broadening of low-energy quasiparticle states by a residual rate γ , which is also roughly proportional to the residual density of states at zero energy $N(0)$. Impurities are thus assumed to “smear out” the nodes of the gap, and therefore inevitably cut off the singular behavior. For example, in the work of Barash et al.[7], no upturn in $\lambda(T)$ at low T is observed if $\gamma > T_{m0}$. In the impurity-dominated regime, a quadratic temperature dependence is generally to be expected[11]. Impurity physics is therefore thought to compete[4] with nonlocal[10] and nonlinear[1] effects

in the Meissner state, and $\lambda(T)$ changes from linear to quadratic below whichever scale is largest.

There may be reasons, however, to doubt results obtained for the penetration depth using the self-consistent T -matrix approximation (SCTMA), which defines a translationally invariant effective medium for the impurity-averaged dirty d -wave superconductor. First, it has been shown to break down in two dimensions[12] and corrections due to weak localization and correlated order parameter response have been under intense investigation recently.[13] Secondly, as with any effective medium theory, it must break down when impurities are sufficiently isolated. Finally, there are clear indications that single impurity bound states in unconventional superconductors are analogous in some respects to surface Andreev states.[14] Here we point out that under some circumstances isolated strong impurities can themselves make singular contributions to the penetration depth and other thermodynamic quantities. While we can present only estimates for the effect of a thermodynamically finite density of dilute impurities, we perform an exact calculation for the current response of a d -wave superconductor in the presence of a single strong scatterer.

Current response for single impurity. We consider a pure d wave superconductor described by Nambu propagator $\underline{G}_{\mathbf{k}}^0(\omega) = (i\omega_n\tau_0 + \xi_{\mathbf{k}}\tau_3 + \Delta_{\mathbf{k}}\tau_1)/D_{\mathbf{k}}$, where $D_{\mathbf{k}} \equiv \omega_n^2 + \xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2$, $\xi_{\mathbf{k}} \equiv \epsilon_{\mathbf{k}} - \mu$ is the 1-electron spectrum measured relative to the Fermi level, and the τ_i are Pauli matrices. The d -wave order parameter on the model cylindrical Fermi surface parametrized by angle ϕ is $\Delta_{\mathbf{k}} = \Delta_0 \cos 2\phi$. In the system with one single δ -function impurity of strength V_0 located at position \mathbf{R} , the Green’s function is exactly given by

$$\underline{G}_{\mathbf{k}\mathbf{k}'}(\omega) = \underline{G}_{\mathbf{k}}^0(\omega)\delta_{\mathbf{k}\mathbf{k}'} + e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}}\underline{G}_{\mathbf{k}}^0(\omega)\underline{T}(\omega)\underline{G}_{\mathbf{k}'}^0(\omega), \quad (1)$$

where \underline{T} is the exact T -matrix for the impurity. We now ask what the *change* in the current response due to a single impurity is in this system. Note that we intend to study at first only the *linear* response to an external vector potential \mathbf{A} à la Kubo, but in the “unperturbed state” described by the *exact* one-particle eigenstates with the single impurity present. This is simply the usual nonlocal

expression for the current response in Coulomb gauge,

$$\mathbf{J}(\mathbf{r}) = \int d\mathbf{r}' \underline{K}(\mathbf{r}, \mathbf{r}') \mathbf{A}(\mathbf{r}'), \quad (2)$$

with $\underline{K}(\mathbf{r}, \mathbf{r}') = -c/(4\pi\lambda^2(T))\delta(\mathbf{r} - \mathbf{r}') + \delta\underline{K}(\mathbf{r}, \mathbf{r}')$. Here we take $\lambda(T)$ to be the unperturbed London penetration depth of the d -wave superconductor, with pure behavior $\lambda(T) \simeq \lambda_0(1 + (\log 2)T/\Delta_0)$ for $T \ll \Delta_0$ and $\lambda_0 \equiv \sqrt{mc^2/4\pi ne^2}$. The Fourier transform $\delta\underline{K}(\mathbf{p}, \mathbf{q})$ is now the change in response due to the impurity, which may be easily expressed in terms of the exact 1-impurity T -matrix using (1),

$$\begin{aligned} \delta K^{\alpha\beta}(\mathbf{p}, \mathbf{q}) = & -\frac{e^2}{c\mathcal{V}} e^{i(\mathbf{p}-\mathbf{q})\cdot\mathbf{R}} T \sum_{\omega} \sum_{\mathbf{l}} \frac{1}{2} \text{Tr} \\ & \left\{ \mathbf{v}_{\mathbf{l}-\frac{\mathbf{p}}{2}}^{\alpha} \mathbf{v}_{\mathbf{l}-\frac{\mathbf{p}}{2}}^{\beta} \underline{G}_{\mathbf{l}}^0(\omega) \underline{G}_{\mathbf{l}-\mathbf{q}}^0(\omega) \underline{T}(\omega) \underline{G}_{\mathbf{l}-\mathbf{p}}^0(\omega) \right. \\ & + \mathbf{v}_{\mathbf{l}+\frac{\mathbf{q}}{2}}^{\alpha} \mathbf{v}_{\mathbf{l}+\frac{\mathbf{q}}{2}}^{\beta} \underline{G}_{\mathbf{l}+\mathbf{p}}^0(\omega) \underline{T}(\omega) \underline{G}_{\mathbf{l}+\mathbf{q}}^0(\omega) \underline{G}_{\mathbf{l}}^0(\omega) + \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} \\ & \left. \mathbf{v}_{\mathbf{l}+\frac{\mathbf{q}}{2}}^{\alpha} \mathbf{v}_{\mathbf{k}-\frac{\mathbf{p}}{2}}^{\beta} \underline{G}_{\mathbf{k}}^0(\omega) \underline{T}(\omega) \underline{G}_{\mathbf{l}+\mathbf{q}}^0(\omega) \underline{G}_{\mathbf{l}}^0(\omega) \underline{T}(\omega) \underline{G}_{\mathbf{k}-\mathbf{p}}^0(\omega) \right\}, \end{aligned} \quad (3)$$

where ω is an internal fermion Matsubara frequency, \mathcal{V} is the volume of the system, and $\mathbf{v}_{\mathbf{k}} \equiv \partial\epsilon/\partial\mathbf{k}$ is the electron velocity.

We now need to solve (2) together with Maxwell's equations to determine the spatial dependence of the vector potential caused by the combined effects of Meissner screening and impurity scattering. Since we are primarily interested in long-wavelength effects, the perturbation may be considered to be of order $1/N$, where N is the number of atoms in the crystal; we may therefore clearly treat the problem perturbatively, by writing $\mathbf{A}(\mathbf{r}) = \mathbf{A}_0(z) + \delta\mathbf{A}(\mathbf{r})$, where the unperturbed solution is taken to be the London result (we assume $\lambda_0 \gg \xi_0$ for the homogeneous system) $\mathbf{A}_0(z) = \mathbf{A}_0(0) \exp(-|z|/\lambda_0)$. Note $z > 0$ is the coordinate describing the theorist's half-space of superconducting material, and the solution $A(\mathbf{r})$ is extended to unphysical values $z < 0$ as an "image vector potential" to allow a solution by Fourier transform. Specular scattering of quasiparticles from the actual surface is assumed throughout.

To linear order in $\delta\mathbf{A}$, the problem can be cast as a differential rather than integro-differential equation,

$$\nabla^2 \delta\mathbf{A} - \frac{1}{\lambda(T)^2} \delta\mathbf{A} = \frac{4\pi}{c} \int d\mathbf{r}' \delta\underline{K}(\mathbf{r}, \mathbf{r}') \mathbf{A}_0(z') \quad (4)$$

whose solution can be obtained by Fourier transform,

$$\begin{aligned} \delta\mathbf{A}(\mathbf{r}) &= - \sum_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{r}} \frac{\mathbf{F}(\mathbf{q})}{q^2 + 1/\lambda^2} \\ \mathbf{F}(\mathbf{q}) &= \frac{4\pi}{c} \int d\mathbf{r} e^{i\mathbf{q}\cdot\mathbf{r}} \int d\mathbf{r}' \delta\underline{K}(\mathbf{r}, \mathbf{r}') \mathbf{A}_0(z'). \end{aligned} \quad (5)$$

With the expressions (2) and (5) it is clearly straightforward, if tedious, to evaluate the full spatial dependence of the vector potential or the current around the

impurity site. It is clear from physical considerations that the current at any given point in space \mathbf{r} will depend both on the distance from the surface z and on the distance from the impurity $|\mathbf{r} - \mathbf{R}|$. In general, then, the currents and field $\mathbf{B} = \nabla \times \mathbf{A}$ are functions of x, y and z everywhere. We postpone the full evaluation to a subsequent study. At present we would like simply to obtain an estimate of the size of this effect, which we do by examining the perturbation of the component of the field along the initial applied field $\mathbf{B}(0)$ which we take to be along y . The penetration depth is usually *defined*, even in cases where the decay of the fields is not exponential, i.e. nonlocal electrodynamics, as $\lambda_{tot} \equiv \int_0^\infty dz B_y/B_y(0)$. So for our current purposes we will simply adopt this definition and evaluate $B_y(x = y = 0, z)$, i.e. at the transverse position of the impurity $\mathbf{R} = (0, 0, z_0)$. In this approximation we find

$$\frac{\delta\lambda}{\lambda} \simeq \frac{\delta A_x(0) + \int_0^\infty dz \partial_x \delta A_z + \lambda \partial_z \delta A_x(0) - \lambda \partial_x \delta A_z(0)}{A_{0x}(0)} \quad (6)$$

A careful examination of these terms and glance at Eq. (5) shows that the size of $\delta(1/\lambda^2) \simeq 2\delta\lambda/\lambda^3$ is simply set by $\delta\underline{K}(\mathbf{p}, \mathbf{q})$ with $p, q \sim 1/\lambda$, as intuitively expected. Expanding Eq. (3) for $p, q \ll k_F$ and performing the integration over energy $\xi_{\mathbf{k}}$ yields from the first two terms

$$\delta K^{xx}(\mathbf{p}, \mathbf{p}) \simeq \frac{ic}{4\pi\lambda_0^2} T \sum_{\omega} \frac{T_0}{\mathcal{V}} \int_0^{2\pi} d\phi \frac{2\omega\Delta_{\mathbf{k}}^2(12\xi_1^2 + \eta_{\mathbf{p}}^2)}{\xi_1^3(4\xi_1^2 + \eta_{\mathbf{p}}^2)^2}, \quad (7)$$

where $\xi_1 \equiv \sqrt{\omega^2 + \Delta_{\mathbf{k}}^2}$, $T_0 = (\pi N_0)^{-1} G_0/(c^2 - G_0^2)$, with $G_0 = (1/2\pi N_0) \text{Tr} \sum_{\mathbf{k}} \underline{G}_{\mathbf{k}}^0 = (2i\omega/\pi\xi_1 N_0) \mathcal{K}(\Delta_0/\xi_1)$, is the τ_0 component of the T -matrix, and c is the cotangent of the s -wave scattering phase shift ($c = 0$ corresponds to infinitely strong scattering). \mathcal{K} is the complete elliptic integral of the first kind. Note that the third term of (3) contains two factors of T_0^2 and therefore formally of order $1/N^2$; we therefore neglect it in its effect on long-wavelength properties like $\delta\lambda$, although it will contribute to local properties. The quantity $\eta_{\mathbf{p}} \equiv \mathbf{v}_{\mathbf{k}} \cdot \mathbf{p} \simeq v_F^z \cdot \mathbf{p}/\lambda$, where the last approximation follows because the primary spatial gradients are perpendicular to the surface with normal \hat{z} , and because we are interested in typical $p \simeq 1/\lambda$. In Figure 1, we show a numerical evaluation of (7) for three different values of the impurity scattering phase shift. As the scattering approaches the unitarity limit, the perturbation to the penetration depth is seen to diverge with decreasing temperature.

To get an analytical estimate of the upturn in the unitarity limit, we first perform a nodal expansion of the order parameter, $\Delta_{\mathbf{k}} \simeq 2\Delta_0(\phi - \phi_n)$, where $\phi_n \equiv \pi/4, 3\pi/4, \dots$, leading for $T \ll \Delta_0$ to the result

$$\delta K^{xx}(\mathbf{p}, \mathbf{p}) \simeq -\frac{c}{4\pi\lambda_0^2} \frac{N_0^{-1}}{2\pi^2 T \mathcal{V}} \frac{1}{n_0 \log \frac{2\Delta_0}{\pi n_0 T}}, \quad (8)$$

where the infrared divergence in (7) was cut off by $\eta_{\mathbf{p}}$ or $c\Delta_0$, and n_0 is the appropriate minimum Matsubara index $n_0 \equiv \max(\eta_{\mathbf{p}}/\pi T, c\Delta_0/\pi T, 1)$. For a (001)

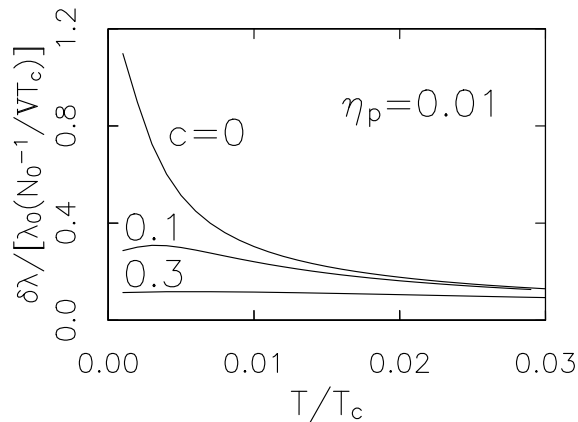


FIG. 1: Normalized change in penetration depth $\delta\lambda/[\lambda_0(N_0^{-1}/\mathcal{V}T_c)]$ due to single isolated impurity vs. normalized temperature T/T_c for three values of the cotangent of the impurity phase shift $c = 0, 0.1, 0.3$. For this plot we took $\eta_p \simeq 0.01T_c$.

surface in the cuprates, $\eta_p \simeq (v_F^z/v_F^\perp)(\xi_0/\lambda_0)\Delta_0 \simeq 10^{-3} - 10^{-4}$, so we get a divergence which goes as $\delta\lambda \sim \lambda_0 E_F/[NT \log(\Delta_0/T)]$. The factor of $1/N$ arises since (8) is proportional to $N_0^{-1}/\mathcal{V} \sim a^3/\mathcal{V}$, where a is the lattice spacing. The estimate holds only for temperatures down to $T_1^* \equiv \max(\eta_p, c\Delta_0)$ at which the divergence is cut off, of order tenths of a Kelvin or less in the cuprates if c is taken to be 0.

Finite density of scatterers. We would now like to extend the above estimate for a single impurity to the case when a finite density of impurities is present. As mentioned above, when brought into proximity these impurities interfere with one another via hybridization of quasiparticle bound state wave functions, leading eventually to an “impurity band” and residual density of states at the Fermi level, at least in 3D[13]. In this situation the SCTMA is the appropriate approximation, and a T^2 behavior in the penetration depth is found rather than an upturn.[11] The conditions for the formation of this band are subtle, and we do not address these questions here.

Intuitively, it seems likely that impurities will act as independent sources of current distortion if they are sufficiently far from one another, but it is not so simple to specify what “sufficiently far” means. We note that both the distortion of the current distribution arising from $\delta K(\mathbf{r}, \mathbf{r}')$ and the impurity bound state wave functions generically decay over lengths of a few ξ_0 . If the typical interimpurity spacing $\ell \equiv n_i^{-1/2}a$ (in 2D) is much greater than ξ_0 , each impurity in a penetration length λ contributes $\delta\lambda$ to the observed $\delta\lambda_{tot}$. On the other hand, even if $\ell \ll \xi_0$, there is a probability $P(R) \simeq \exp(-R^2/2\ell^2)$ that an impurity will find itself with no other impurities within a radius R , if all impurities are randomly distributed. We therefore expect that an *upper bound* to the observable penetration depth upturn in the case of randomly distributed unitarity limit

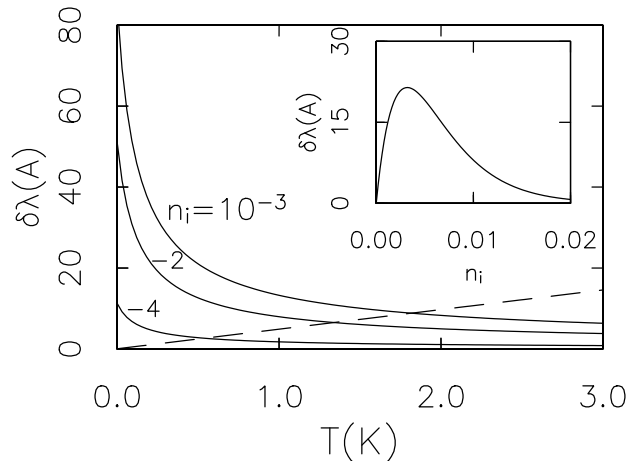


FIG. 2: Change in penetration depth $\delta\lambda_{tot}(\text{\AA})$ due to isolated unitarity limit scatterers vs. temperature $T(K)$ for three impurity concentrations $n_i = 10^{-2}, 10^{-3}, 10^{-4}$. $\Delta_0/T_c = 2.14$, $\eta_p/T_c = 0.001$, $T_c = 100K$. Dashed line: T -variation of pure penetration depth $(\log 2)T/\Delta_0$. Inset: $\delta\lambda_{tot}$ vs. n_i at $T = 1K$.

scatterers will be

$$\delta\lambda_{tot} \simeq \frac{n_i P(\xi_0) E_F}{4\pi^2 \tilde{T} \log(2\Delta_0/\pi\tilde{T})} \lambda_0, \quad (9)$$

with $\tilde{T} = T + T_1^*$. The estimate is an upper bound because we do not currently know how to calculate accurately a geometric factor arising from the contribution of those impurities which are located such that the tails of *nodal* quasiparticle resonant states (which do not decay as $e^{-\xi_0/r}$ but rather as $1/r$ at $\omega = 0$)[15, 16] overlap. This factor will lead to significant hybridization and smearing of the singularity at impurity densities below that given by the criterion above. We nevertheless substitute some numbers into (9) to check for plausibility, taking $E_F/\Delta_0 \simeq 10$, $\lambda = 1500\text{\AA}$, and $\xi_0 = 25\text{\AA}$ for the cuprates. In Figure 2, we plot the results of (9) in laboratory units given these assumptions. It is seen that, within this crude approximation, the size of the upturn expected is not monotonic with impurity concentration, but at a temperature of 1K peaks around $n_i \simeq 10^{-3}$. The position T_2^* of the minimum in $\lambda_{tot}(T)$ will now be set by comparing the impurity-induced change in λ with that due to thermally excited quasiparticles, $\delta\lambda(n_i, T_2^*) \sim T_2^* \lambda_0/\Delta_0$; for impurity concentrations of $n_i = 10^{-3} - 10^{-2}$, this temperature will be of order 1-2K, as seen in Figure 2.

The size of the increases predicted seem quite reasonable, and are of the same order of magnitude as the upturns seen in the work of Bonn et al.[9] and Carrington et al.[8] Although the latter authors observed a substantial increase in the size of the signal when the proportion of (110) surface in the given sample was maximized, indicative of an Andreev surface bound state contribution, there was a substantial signal even in samples with only (100) surfaces, where surface bound states should not ex-

ist. Although the authors' suggestion that this result is due to (110) faceting in these samples is possible, the mechanism we suggest may also be present.

While the estimate (9) is based on the assumption of randomly distributed impurities, it is important to recognize that in real systems clustering will take place. In this case even a relatively disordered system may have significant numbers of isolated impurities or isolated atomic-scale clusters which give rise to a singular current response. In this case we might expect significant sample-to-sample variation in $\delta\lambda$ in samples with identical average concentration n_i . This appears to be precisely the effect found by Bonn *et al.* in their measurements on YBCO single crystals with 0.31% Zn[9].

Magnetic field. Since the penetration depth upturn in the case considered here is due to the large number of quasiparticle excitations near the nodal directions, as is the similar upturn in the case of Andreev surface states, we might expect any physical effect which smears the gap nodes to cut off the upturn. In particular, the orbital coupling to an applied magnetic field (nonlinear electrodynamics) will suppress the upturn as it does in the Andreev case[7]. We need only add the Doppler shift of the quasiparticle energy in any of the expressions above, $i\omega \rightarrow i\omega + \mathbf{v}_s \cdot \mathbf{k}$, where \mathbf{v}_s is the local superfluid velocity. A typical shift $v_s k_F \simeq (H/H_0)\Delta_0$, where H is the applied field and $H_0 = 3\Phi_0/(\pi^2\xi_0\lambda_0)$ is of the order of the thermodynamic critical field, and the effect of the field may be included approximately by generalizing $\tilde{T} \rightarrow T + T_1^* + (H/H_0)\Delta_0$ in (9). We postpone a more quantitative study of the field dependence to a later work.

Conclusions. We predict that a *d*-wave superconduc-

tor with isolated strong nonmagnetic impurities should exhibit an upturn in the penetration depth varying as $1/T \log T$ below a temperature scale set by the disorder in the system and above one set by the bulk penetration depth or the scattering phase shift. This effect may have contributed to upturns already observed in experiments where Andreev surface states, which produce a similar effect, are not indicated[8, 9]. The physical origin of the upturn in both cases is the depletion of the supercurrent at low T in low-energy bound states, but the impurity-induced upturn is independent of surface geometry. We argue that the magnitude of the effect should have a characteristic dependence not only on the concentration of impurities, but on the exact nature of the statistical distribution of impurities in the sample. We emphasize that the estimates presented here are merely a crude plausibility argument that if such upturns are observed at low temperatures, they could arise from singular current response of local defects in the crystal, and that it will be useful to study the dependence on disorder. Our work also allows in principle an exact calculation of the local current flow around an impurity; it will be interesting to see how the singular quasiparticle currents are distributed in the neighborhood of the impurity site, and whether these features can be detected by STM.

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